REPORT

DETERMINATION OF THE DENSITY (LIQUID) OF

[redacted]

NOTOX Project 338579
NOTOX Substance 111834/C

CONFIDENTIALITY STATEMENT

This report contains the unpublished results of research sponsored by [redacted] Chemicals B.V. Reproduction, issue or disclosure to third parties in any form is not permitted without prior written authorisation from the sponsor.

STATEMENT OF GLP COMPLIANCE

NOTOX B.V., 's-Hertogenbosch, The Netherlands

The study described in this report has been correctly reported and was conducted in compliance with the most recent edition of:

The OECD Principles of Good Laboratory Practice

which are essentially in conformity with:

The United States Food and Drug Administration. Title 21 Code of Federal Regulations Part 58.

The United States Environmental Protection Agency (FIFRA). Title 40 Code of Federal Regulations Part 160.

The United States Environmental Protection Agency (TSCA). Title 40 Code of Federal Regulations Part 792.

Study Director

[redacted]

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Date: March 27, 2002.

Management

[redacted]tical & Physical Chemistry

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Date: March 27, 2002

QUALITY ASSURANCE STATEMENT

NOTOX B.V., 's-Hertogenbosch, The Netherlands

This report was audited by the NOTOX Quality Assurance Unit to ensure that the methods and results accurately reflect the raw data.

The dates of Quality Assurance inspections and audits are given below.
During the on-site inspections procedures applicable to this type of study were inspected.

DATES OF QAU INSPECTIONS/AUDITS	REPORTING DATES
on-site inspection (s)	
03-Dec-2001 to 05-Dec-2001 (process)	11-Dec-2001
protocol inspection (s)	
14-Jan-2002 (study)	14-Jan-2002
report audit (s)	
14-Mar-2002 (study)	14-Mar-2002

Head of Quality Assurance
[redacted].

Date: 28-3-02 .

SUMMARY

The determination of the density (liquid) was based on the EEC-Directive 92/69 EEC, A.3 "Relative density" (1992) and on the OECD Guideline no. 109 "Density of liquids and solids" (1995).

The density of the liquid test substance [redacted] is 1.16 g/cm^3 (1.16*10^3 kg/m^3).
A glass pycnometer with a nominal volume of 10 ml was used.
Temperature of measurement was 20.0 ± 0.5°C.

The D_4^{20} is 1.16.

PREFACE

Sponsor	[redacted]
Study Monitor	[redacted] SHERA, Regulatory Affairs
Testing Facility	NOTOX B.V. Hambakenwetering 7 5231 DD 's-Hertogenbosch The Netherlands
Study Director	[redacted]
Study Plan	Start : 06 February 2002 Completed : 06 February 2002

TEST SUBSTANCE

Identification	
Chemical name	[redacted] and [redacted]
Description	Clear colourless liquid
Batch	1510-14
Purity	See Certificate of Analysis
Test substance storage	In refrigerator in the dark
Stability under storage conditions	Stable
Expiry date	01 January 2003

The sponsor is responsible for all test substance data unless determined by NOTOX.

Note: **Don't heat up the test substance above 50°C**

PURPOSE

The purpose of the study was to determine the density of the test substance at a specific temperature by means of a pycnometer.

GUIDELINES

The study procedure described in this report is based on the following guidelines:

Organization for Economic Co-operation and Development (OECD), OECD guidelines for Testing of Chemicals, guideline No. 109: "Density of liquids and solids", July 27, 1995.

European Economic Community (EEC), EEC-Directive 92/69 EEC, Part A, Methods for the determination of physico-chemical properties, A.3 "Relative density", EEC Publication No. L383, December 1992.

ARCHIVING

NOTOX B.V. will archive the following data for at least 10 years: protocol, report, test substance reference sample and raw data. Thereafter, no data will be withdrawn without the sponsor's written consent.

TEST SYSTEM AND RATIONALE

Test system	A pycnometer with a ground-in thermometer and a capillary side-tube and with a volume of 10 ml.
Weighings	An analytical balance with an accuracy of 0.1 mg.
Conditions	All manipulations were performed at 20.0 $\pm$ 0.5°C with equipment having the same temperature.
Rationale	Recognized by the international guidelines as recommended test system (EEC, OECD).

PERFORMANCE OF THE TEST

First the volume of the pycnometer was determined (in duplicate); the pycnometer was weighed dry and empty (A), filled with Milli-Q water (Millipore Corp., Bedford, MA, USA), thoroughly dried on the outside and weighed again (B).

The density of the liquid test substance was calculated from the difference in weight between the full (C) and empty pycnometer (mean A) and its known volume (mean D). This procedure was repeated until reproducible results (deviation in the density < 0.01 g/cm^3) were obtained.

DATA HANDLING

Definitions:

The density of a substance is the quotient of the mass m and the volume v of that substance at a specific temperature.

density = m/v

SI unit in kg/m^3. One gram per cm^3 corresponds with 1000 kg/m^3.

The D_4^{20} : The ratio between the mass of a volume of the test substance, determined at 20°C, and the mass of the same volume of water, determined at 4°C. The relative density has no dimension.

Calculations:

The following calculations were performed:

(B - A) / SMW = D

$(C - A_{mean}) / D_{mean} = E$ density of the test substance at the test temperature (g/cm^3)

A = weight of the empty pycnometer (g)
B = weight of the pycnometer with Milli-Q water (g)
C = weight of the pycnometer with the test substance (g)
D = volume of the pycnometer (cm^3)
SMW = density of water at the test temperature (g/cm^3) (CRC Handbook of Chemistry and Physics, 1981)

RESULTS

The test was performed in duplicate. Individual results are shown in Table 1. Measurements and calculations are shown in the Appendix.

Table 1 Determinations of the density of [redacted]

Measurement	Temperature of measurement [°C]	Density [g/cm^3]
1	20.0	1.160
2	20.0	1.161
mean:		1.16

In conclusion, the density of [redacted] is 1.16 g/cm^3 ($1.16*10^3$ kg/m^3).

The D_4^{20} is 1.16.

APPENDIX

Individual measurements		
	Experiment 1	Experiment 2
PYCNOMETER EMPTY (A)	25.9025 g	25.9027 g
TEMP. MILLI-Q WATER	20.0°C	20.0°C
PYCNOMETER + MILLI-Q WATER (B)	35.6667 g	35.6709 g
TEMP. TEST SUBSTANCE	20.0°C	20.0°C
PYCNOMETER + TEST SUBSTANCE (C)	37.2535 g	37.2634 g

Calculations

1. SMW (resulting from the test temperature) = 0.9982 g/cm^3

2. Volume pycnometer = D = (B - A) / SMW

   Exp. 1 : D = 9.7818 cm^3
   Exp. 2 : D = 9.7858 cm^3
   Mean D= 9.7838 cm^3

3. Density test substance = (C - A_{mean}) / D_{mean}

   Exp. 1 : density = 1.160 g/cm^3
   Exp. 2 : density = 1.161 g/cm^3
   Mean density = 1.16 g/cm^3

CERTIFICATE OF ANALYSIS

[redacted]

Certificate of Analysis [redacted]

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Product name : [redacted]

Chemical name : [redacted])

Batch number : **1510-14**

Test results:

Method	Analysis of	Unit	Result *1
Jo/72.11, [redacted]	[redacted] *See page 2 for a specification*		
J20010792	[redacted]		
	[redacted]	% m/m	2.0 (± 0.3)
Amp/88.9	[redacted]	% m/m	2.6 (± 0.3)
J20010792	Unidentified impurities	% m/m	0.5 (± 0.2)

*1 bracketed values are estimated 95% confidence intervals

File code : **TNA-2001007**

Analytical documentation : 20010792

Authorized by

Name : [redacted]
Function : Section Head, Analytical Research Department
Date : October 25, 2001

Signature :

[redacted]

[redacted]

Certificate of Analysis [redacted]

[redacted]

structure	% m/m
[redacted] (Type IV) IUPAC : [redacted]	18.6
[redacted] (Type III) IUPAC : [redacted]	7.9
[redacted]	2.1

[redacted]